

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in this application.

Listing of Claims:

Claims 1-11 (cancelled)

12. (withdrawn) A method for evaluating the potential of a chemical entity to associate with:

a) a molecule or molecular complex comprising a binding pocket defined by structure coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å,

said method comprising the steps of:

(i) employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

(ii) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket; and

(iii) outputting said quantified association to a suitable output hardware.

13. (withdrawn) The method according to claim 12, wherein said method evaluates the potential of chemical entity to associate with:

a) a molecular or molecular complex comprising a binding pocket defined by the structural coordinates of JNK3 amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207, according to Figure 1; or

b) a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

14. (withdrawn) The method according to claims 12 or 13, wherein said method evaluates the potential of a chemical entity to associate with a molecule or molecular complex:

a) defined by the set of structure coordinates for JNK3 amino acids, as set forth in Figure 1; or

b) a homologue of said molecule or molecular complex having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

Claim 15 (cancelled)

16. (withdrawn-currently amended) A method for designing an inhibitor of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule, comprising the step of:

using the atomic coordinates in Figure 1A, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, which describe [[a]] an active site binding pocket of the unphosphorylated JNK3 α , to design or select said inhibitor, where said active site binding pocket comprises the amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206.

17. (withdrawn-currently amended) The method according to claim 16, wherein said active site binding pocket additionally comprises the amino acids Ile77, Cys79, Ala80, Val90, Ile92, Lys94, Leu95, His104, Arg107, Ser125, Leu144, Val145, Leu153, Cys154, Asp189, Pro192, Ile195, Val197, Lys204 and Asp207.

Claim 18 (cancelled)

19. (withdrawn-currently amended) The method according to claims 16 or 17, wherein ~~[[the]]~~ a potential inhibitor is contacted with said unphosphorylated JNK3 α molecule to determine the ability of said potential inhibitor to ~~interact~~ associate with the unphosphorylated JNK3 α molecule.

20. (withdrawn-currently amended) A method for designing an inhibitor of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule comprising the steps of:

a) producing a crystal of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule and a chemical entity, wherein said unphosphorylated JNK3 α molecule contains an N-terminal deletion of 39 amino acids;

b) determining the three-dimensional atomic coordinates of amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 of [[a]] an active site binding pocket of the unphosphorylated JNK3 α molecule by X-ray diffraction of the crystal;

c) using said coordinates, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to design or select said inhibitor.

21. (withdrawn-currently amended) The method according to claim 20, further comprising the step of contacting [[said]] a potential inhibitor with said unphosphorylated JNK3 α molecule to determine the ability of said potential inhibitor to ~~interact~~ associate with said unphosphorylated JNK3 α molecule.

22. (withdrawn-currently amended) The method according to claim 20, wherein said unphosphorylated JNK3 α molecule further contains a C-terminal deletion of 20 amino acids.

23. (currently amended) A method for identifying an inhibitor of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule, comprising the step of:

a) using the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1A \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a JNK3 α active site binding pocket;

b) employing said three-dimensional structure to design or select ~~said potential agonist or antagonist~~ a potential inhibitor;

c) synthesizing said ~~agonist or antagonist~~ potential inhibitor; and

d) contacting said ~~agonist or antagonist~~ potential inhibitor with said molecule to determine the ability of ~~said~~

~~potential agonist or antagonist~~ a potential inhibitor to
~~interact~~ associate with said molecule.

24. (currently amended) The method according to claim 23, wherein the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1A \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate said three-dimensional structure of the molecule comprising a JNK3 α active site binding pocket.

25. (currently amended) A method for identifying an inhibitor of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule, comprising the steps of:

a) producing a crystal of an unphosphorylated JNK3 α (c-Jun N-terminal kinase 3 α) molecule and a chemical entity, wherein said unphosphorylated JNK3 α molecule contains an N-terminal deletion of 39 amino acids;

b) determining the three-dimensional atomic coordinates of amino acids Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 of [[a]] an active site binding pocket of the unphosphorylated JNK3 α molecule by X-ray diffraction of the crystal;

c) using the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Val78, Ala91, Lys93, Glu111, Ile124, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Gln155, Lys191, Ser193, Asn194, Val196 and Leu206 according to Figure 1A \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, to generate a three-dimensional structure of molecule comprising a JNK3 α active site binding pocket;

d) employing said three-dimensional structure to design or select ~~said potential agonist or antagonist~~ a potential inhibitor;

e) synthesizing said ~~agonist or antagonist~~ potential inhibitor; and

f) contacting said ~~agonist or antagonist~~ potential inhibitor with said molecule to determine the ability of said

~~potential agonist or antagonist~~ potential inhibitor to
~~interact~~ associate with said molecule.

26. (currently amended) The method according to claim 25, wherein the atomic coordinates of Ile70, Gly71, Ser72, Gly73, Ala74, Gln75, Gly76, Ile77, Val78, Cys79, Ala80, Val90, Ala91, Ile92, Lys93, Lys94, Leu95, His104, Arg107, Glu111, Ile124, Ser125, Leu144, Val145, Met146, Glu147, Leu148, Met149, Asp150, Ala151, Asn152, Leu153, Cys154, Gln155, Asp189, Lys191, Pro192, Ser193, Asn194, Ile195, Val196 Val197, Lys204, Leu206 and Asp207 according to Figure 1A \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, are used to generate said three-dimensional structure of the molecule comprising a JNK3 α active site binding pocket.